IJCLab
Irène Joliot-Curie
Laboratoire de Physique des 2 Infinis

E&E Energie & Environement
Energy & Environment

Soutenance de thèse

Vinicius Oliveira Cavalcanti

Vendredi 20 janvier 2023, 14h00

Auditorium Joliot-Curie, Bâtiment 100

Study of helium accumulation at oxide-iron interfaces in fusion-based materials

Summary:

Oxide dispersion strengthened (ODS) steels are excellent candidates for future nuclear reactor applications (fission and fusion). They perform well at high pressure, temperature (T) and irradiation conditions and have higher creep performance at elevated T. It is also believed that the oxide nanoparticles dispersed in the ferritic matrix may act as trapping centres for helium (He) and avoid cracking due to this gas accumulation inside the matrix. However, the influence of this dispersion and the mechanism of He behaviour and diffusion in the steel is not yet well known.

This thesis's objective is a thorough analysis of the He behaviour and diffusion in all the main components of the ODS steels: iron (Fe) and iron-chromium alloy (FeCr) for the matrix, yttrium oxide (Y_2O_3 or yttria) for the nanoparticles, and their interface. For this, both theoretical and experimental methods are employed in a complementary way. The first consists of theoretical simulations using density functional theory (DFT), molecular dynamics (MD) and kinetic Monte Carlo (KMC). The second is based on He ion implantations, followed by experimental characterisations of the He behaviour by transmission electron microscopy (TEM) and thermo-desorption spectrometry (TDS). The samples employed were high-purity Fe and Fe10Cr, high-purity Y_2O_3 with nanometric and micrometric grains, and a model bilayer Y_2O_3/Fe10Cr representing the interface.

Fe was modelled using DFT and KMC to calculate the He diffusion coefficient expression. It was seen that He diffuses fast inside Fe with an activation energy of 0.06 eV. The presence of chromium did not change the results significantly, so it was not considered in the following. Inversely, vacancies played a vital role by reducing the diffusion, with an activation energy of 2.35 eV. This comes from the Fe vacancy accommodation power, where a monovacancy may accommodate 10 to 20 He atoms, responsible for the He bubbles nucleation process. This result was observed using TEM. The bubbles observed were tiny with roughly 0.7 nm radius, and no significant difference between Fe10Cr and pure Fe was observed. Finally, the TDS evidenced 2 main mechanisms of He desorption, depending on the fluence of implanted He. Cr played a role by delaying the He desorption. A model was developed based on the DFT that fitted well with the experimental data, corroborating the different methods.

The same methods were applied to Y_2O_3. The higher He insertion sites showed roughly 1000 times lower interstitial diffusion than Fe at 1000 K. He atoms tend to be distributed inside the material instead of in a specific site. We could not observe any He bubbles using TEM, possibly due to the He dispersion, so it was too small for our microscope (below 1 nm diameter). With TDS, we showed a simple mechanism where He release may come primarily from leaving the different interstitial sites. The nanometric grains showed similar behaviour to the micrometric ones, with earlier desorption, probably coming from the grain boundaries diffusion. A model was also developed based on the TDS data.

The interface between the materials was modelled using DFT, with an optimised interface model with vacuum, the 2 outermost layers frozen, and 6 layers for Fe and 4 for Y_2O_3. Then, the He insertion energies and migration pathways were calculated, showing the most stable configuration to be the one in Y_2O_3 next to the interface. Experimentally, the interface bilayer model was implanted with He at different T. The He bubbles are bigger around the interface, primarily visible around them and Fe. They tend to be slightly bigger with the T increase.

In summary, He behaviour was characterised for the different components of ODS steels. He tends to be more mobile in Fe (except when its vacancies trap it), diffuses slower in Y_2O_3, being dispersed inside it, and is more stable around the interface. This behaviour tends to confirm the potential for ODS steels to be used in future reactors.

Direction de thèse: Aurélie Gentils et Jérôme Roques

IJCLab - Laboratoire de Physique des 2 Infinis **Irène Joliot-Curie**
Bâtiment 100 - 15 rue Georges Clémenceau - 91405 Orsay cedex - France
UMR 9012, CNRS, Université Paris-Saclay, Université de Paris

cnrs
université PARIS-SACLAY
Université de Paris

www.ijclab.in2p3.fr